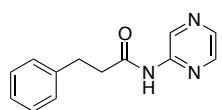


Friedel-Crafts Acylation with Amides

Erum K. Raja^a, Daniel J. DeSchepper^a, Sten O. Nilsson Lill^b, and Douglas Klumpp^{a,*}

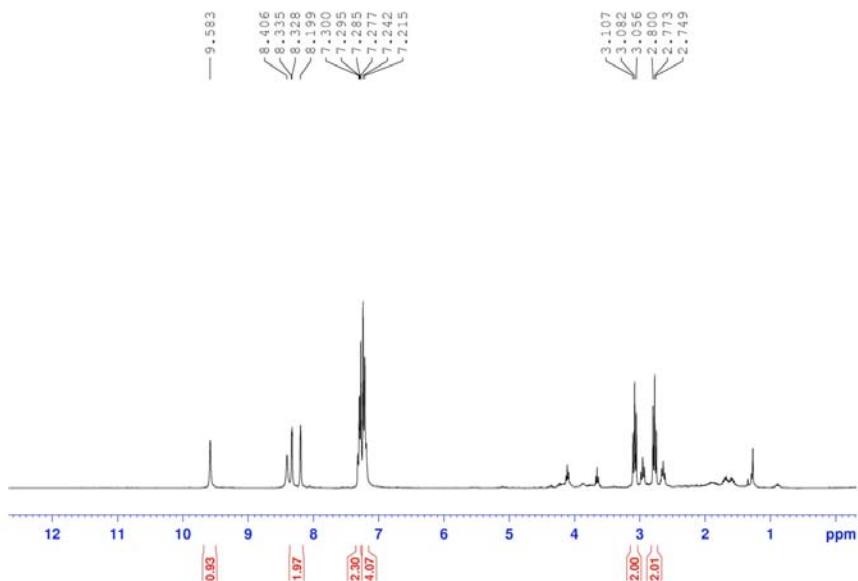
^aDepartment of Chemistry and Biochemistry, Northern Illinois University, Dekalb IL 60115, United States. ^bDepartment of Chemistry, University of Gothenburg, SE-412 96 Gothenburg, Sweden.

| | |
|-------------|---|
| S-1 | Index |
| S-2 – S-7 | ¹ H NMR and ¹³ C NMR spectra of unknown compounds |
| S-8 – S-10 | References to known compounds |
| S-11 | Recent benzophenone preparations |
| S-12 – S-13 | Computational methods and references to these |
| S-13 | Table S1. Calculated occupancy numbers |
| S-14 – S-29 | Cartesian coordinates of compounds discussed in the manuscript |

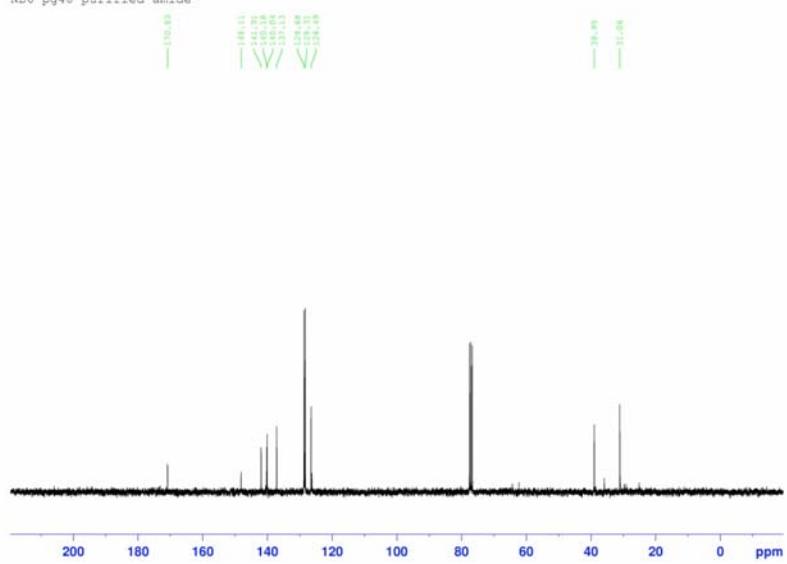


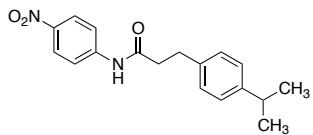
1b (CDCl₃)

NB6 pg40 purified amide

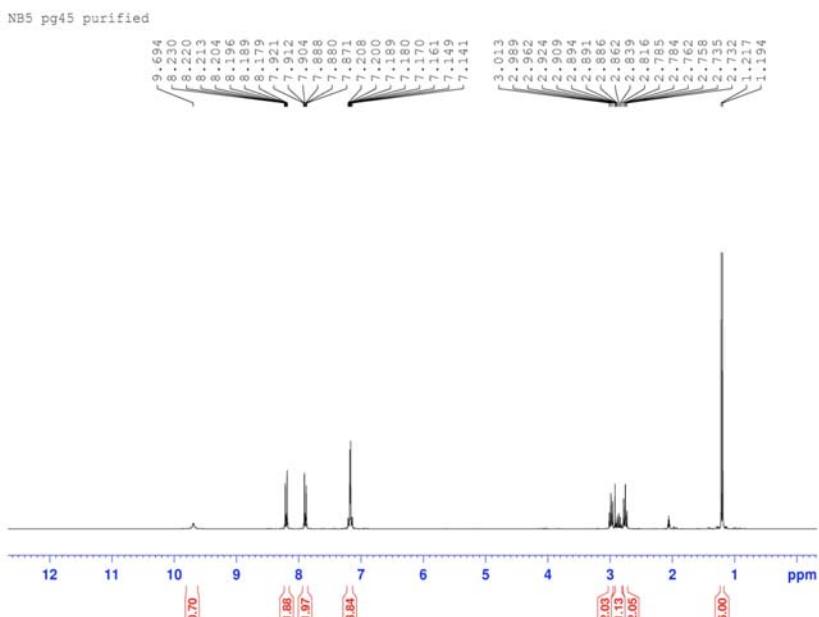


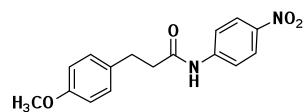
NB6 pg40 purified amide



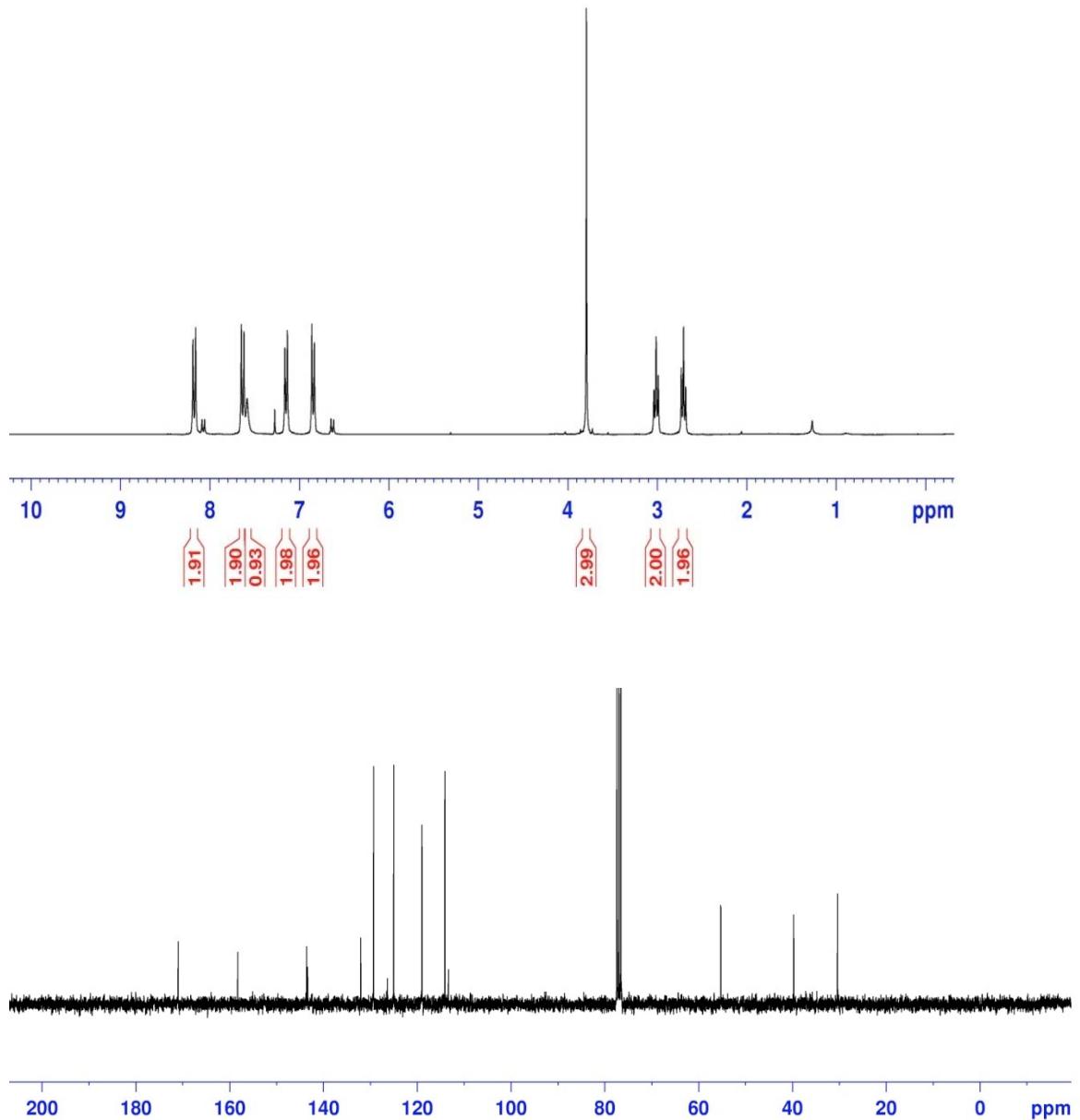


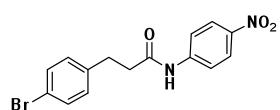
3 (d₆-acetone)



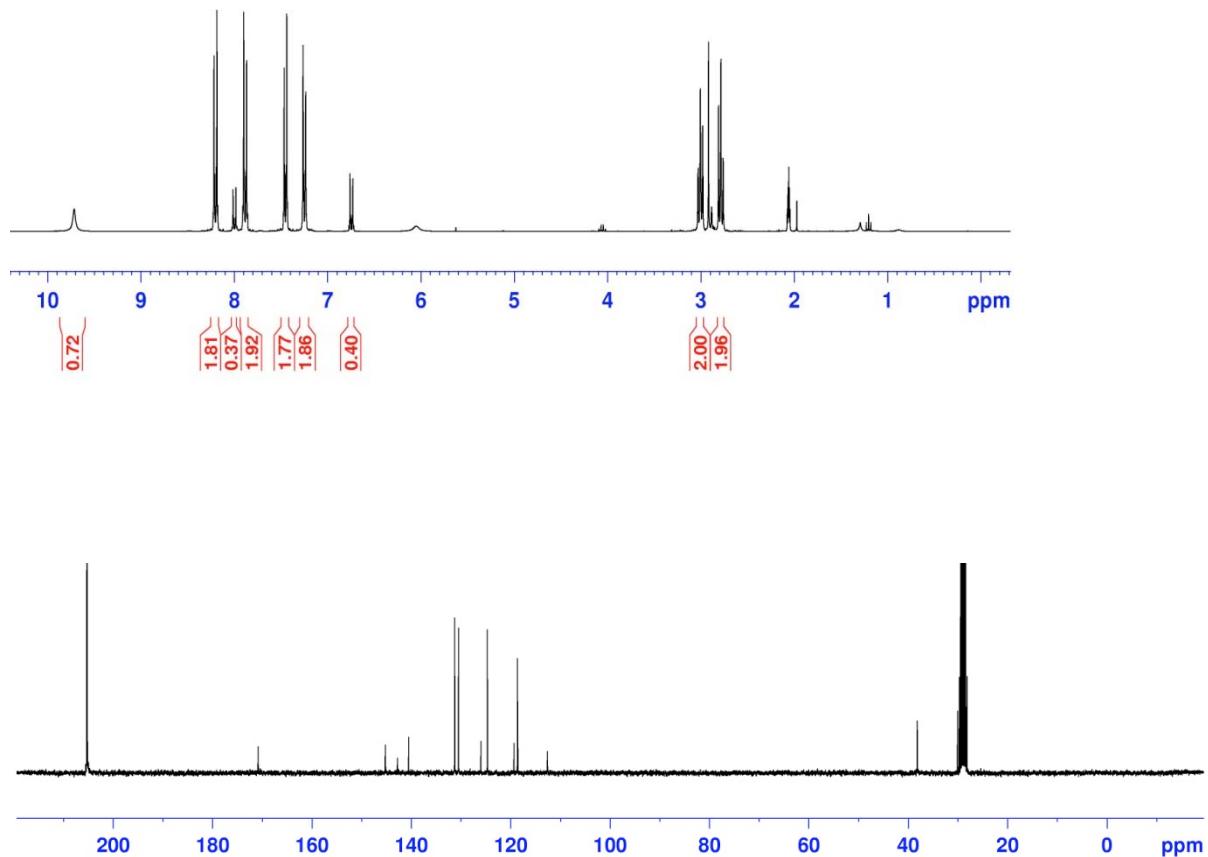


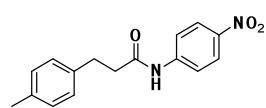
5 (CDCl_3)



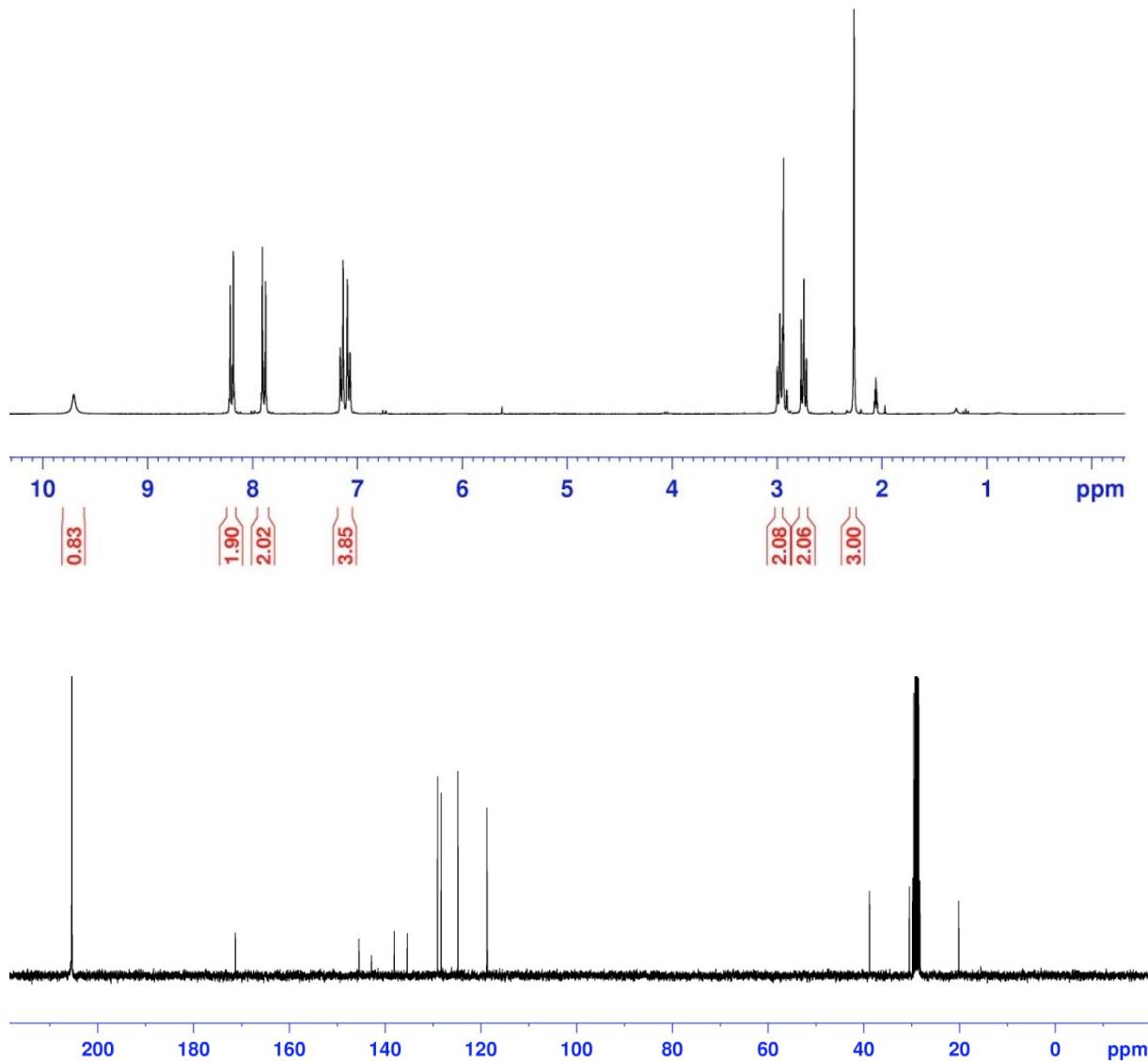


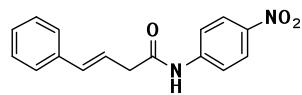
6 (d_6 -acetone)



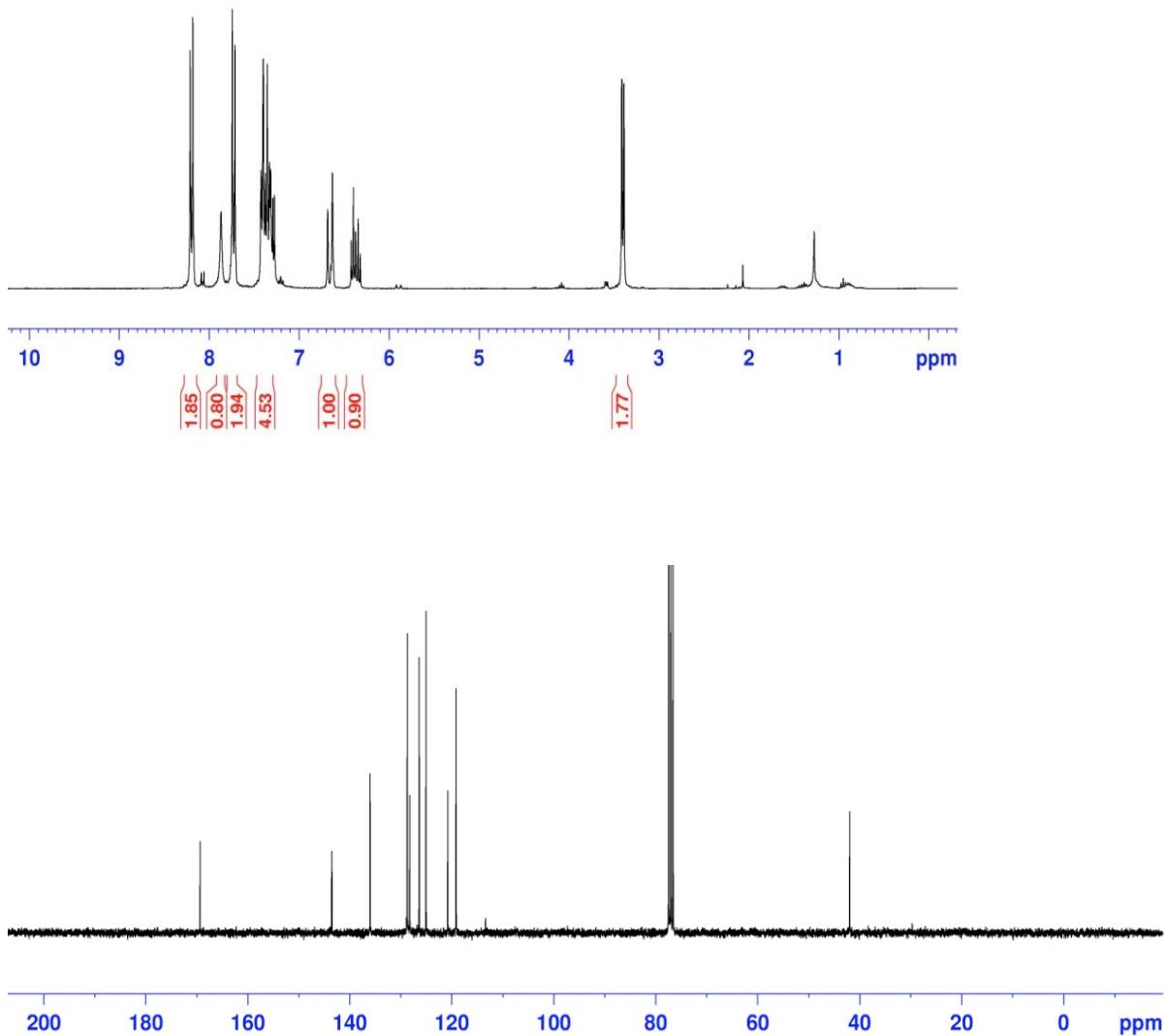


4 (d_6 -acetone)



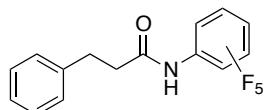


14 (CDCl_3)

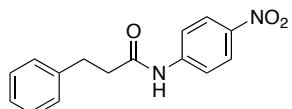


Compounds **2**, **9-12**, **16-19**, and **23** are available from commercial suppliers. These products, as well as the known compounds below, were fully characterized and show analytical data consistent with published data.

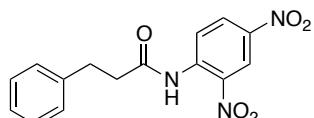
Known compounds and literature citations:



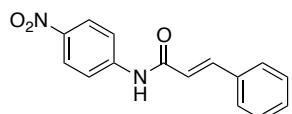
- 1a** Wasa, M.; Engle, K. M.; Yu, J.-Q. *J. Am. Chem. Soc.* **2009**, *131*, 9886.



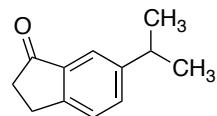
- 1c** Upadhyaya, R. S.; Kulkarni, Girish M.; Vasireddy, N. R.; Vandavasi, J. K.; Dixit, Shailesh S.; Sharma, V.; Chattopadhyaya, J. *Bioorg. Med. Chem.* **2009**, *17*, 4681



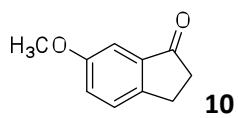
- 1d** Miyashita, M.; Shiina, I.; Mukaiyama, T. *Bull. Chem. Soc. Jpn.* **1994**, *67*, 210.



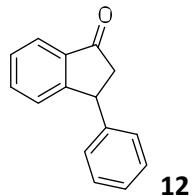
- 7** Weidner-Wells, Michele A.; Fraga-Spano, Stephanie A.; Turchi, Ignatius J., *J. Org. Chem.*, **1998**, *63*(18), 6319-6328.



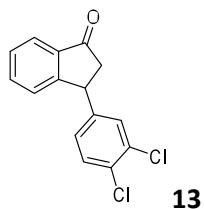
- 8** Matasi, J. J.; Caldwell, J. P.; Hao, J.; Neustadt, B.; Arik, L.; Foster, C. J.; Lachowicz, J.; Tulshian, D. B. *Bioorg. Med. Chem. Lett.* **2005**, *15*, 1333.



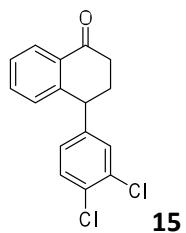
Noureldin, N.; Zhao, D.; Lee, D.; *J. Org. Chem.*, **1997**, 62(25), 8767-8772.



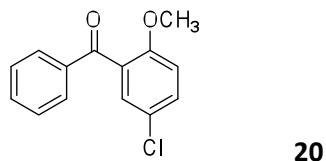
Kangani, C.; Day, B.; *Org. Lett.*, **2008**, 10(13), 2645-2648.



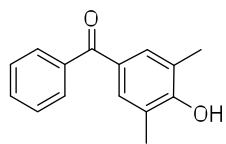
Rendy, R.; Zhang, Y.; McElrea, A.; Gomez, A.; Klumpp, D. *J. Org. Chem.*, **2004**, 69(7), 2340-2347.



Xinbo, W.; Zhigang, W.; *Tetrahedron*, **2011**, 67(19), 3406-3411.

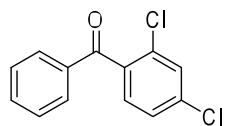


Xing, D.; Guan, B.; Cai, G.; Fang, Z.; Yang, L.; Shi, Z.; *Org. Lett.*, **2006**, 8(4), 693-696.



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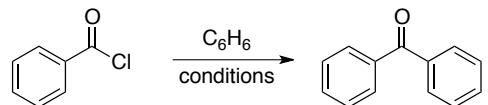
Vazzana, I.; Budriesi, R.; Terranova, E.; Ioan, P.; Urgenti, P.; Tasso, B.; Chiarini, A.; Sparatore, F.; *J. Med. Chem.*, **2007**, 50(2), 334-343.



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Haddach, M.; McCarthy, J.; *Tetrahedron Lett.*, **1999**, 40(16), 3109-3112.

Recent reports of the reaction of benzoyl chloride to form benzophenone:



| Yield | Conditions | Reference |
|-------|--|--|
| 80% | FeCl ₃ on K-10 clay | <i>Ind. J. Chem., Sec. B</i> 2005 , 44B, 188-192 |
| 81% | InCl ₃ , ionic liquid solvent, 80°C | <i>Chem. Comm.</i> 2005 , 903-905 |
| 84% | AgNO ₃ , EtOH | <i>Synth. Comm.</i> 2011 , 41, 953-955 |
| 90% | Ga(ONf) ₃ | <i>Synlett</i> 2000 , 403-405 |
| 87% | FeCl ₃ , H ₃ PO ₄ , KCl, sol-gel | <i>J. Mol. Cat. A: Chem.</i> 2005 , 241, 151-155 |
| 90% | Al(OTf) ₃ , C ₆ H ₅ NO ₂ | <i>Bull. Korean Chem. Soc.</i> 2010 , 31, 3156-3158 |
| 91% | AlCl ₃ on silica gel | <i>Chinese Chem. Lett.</i> 2010 , 21, 1395-1398 |
| 90% | FeCl ₄ NBu ₄ | <i>Chem. Lett.</i> 2008 , 37, 844-845 |
| 94% | Fe ₂ O ₃ | <i>Adv. Synth. Catal.</i> 2010 , 352, 3031-3044 |
| 97% | FeCl ₃ , ionic liquid solvent | <i>Catal. Comm.</i> 2007 , 8, 1834-1837 |
| 50% | ZnO | <i>J. Org. Chem.</i> 2004 , 69, 6953-6956 |

Computational Methods:

In our mechanistic studies, the intermediates and transition states were studied using density functional theory (DFT). Geometries for these structures were initially optimized in the gas phase at the M06/6-31G(d) level of theory¹ using Jaguar.² Gibbs' free energy corrections (ΔG) were calculated, and structures were verified to be minima or transition states by inspection of the number of imaginary frequencies. In a second step, single-point energies of the optimized structures were calculated using M06/cc-pVTZ(-f),^{3,4} giving a basis set correction term (ΔBS). In a final step, solvent phase single point calculations were done at the M06/6-31G(d) level of theory. Using a Poisson-Boltzmann solver as implemented in Jaguar,⁵ electrostatic solvation effects from the surroundings were calculated using the SCRF method with CF₃SO₃H as a solvent (dielectric constant = 77.4, probe radius = 2.5985274).^{6,7} The free energy (ΔG) and basis set correction terms (ΔBS) were added to the solution phase energy. In some selected cases, geometries were also optimized in solution phase to investigate its influence on the optimized geometry. To verify the M06-calculated reaction energy (+15.9 kcal/mol) between compound **25** and **26**, this was also calculated using a ΔBS from single-point calculations using B3LYP/cc-pvtz(-f) (+15.3), LMP2/cc-pvtz(-f) (+11.0). By performing a LMP2/6-31G*(d) calculation resulting in a value of +9.0 kcal/mol, and comparing with the value from the larger basis set, an estimate of the basis set dependence for wavefunction calculations was made. This was added to a CCSD(T)/6-31G(d) level calculation (+11.3 kcal/mol) resulting in an estimated value for the reaction energy at the CCSD(T)/cc-pvtz(-f) level of theory to be +13.3 kcal/mol, in reasonable agreement with the M06-calculated value. This indicates that the M06-value of +15.9 kcal/mol represents an upper limit to the reaction energy. CCSD(T) calculations were done using Gaussian 09.⁸ Orbital occupancy numbers were calculated using NBO 5.0⁹ as implemented in Jaguar.

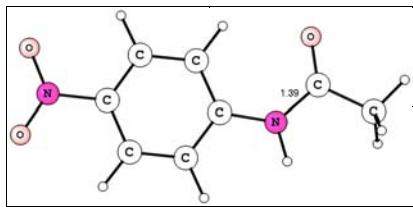
1. Zhao, Y.; Truhlar, D. *Theor. Chem. Acc.* **2008**, *120*, 215–241.
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8. Gaussian 09, Revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.;

Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

9. NBO 5.0. Glendening, E. D.; Badenhoop, J. K.; Reed, A. E.; Carpenter, J. E.; Bohmann, J. A.; Morales, C. M.; Weinhold, F. (Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, 2001); <http://www.chem.wisc.edu/~nbo5>

Table S1. Calculated occupancy numbers

| Compound | Occupancy number (in electrons) | | |
|-----------|---------------------------------|------------------------|---------------------------|
| | Amide n _N | Amide π* _{CO} | Amide σ* _{NC(O)} |
| | 1.68 | 0.27 | 0.08 |
| 24 | | | |
| | 1.68 | 0.24 | 0.09 |
| 16 | | | |
| | 1.88 | 0.17 | 0.11 |
| 28 | | | |
| | 1.99 | 0.08 | 0.37 |
| 33 | | | |



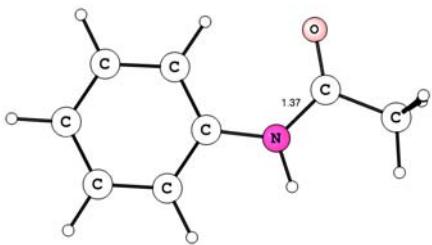
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Cartesian Coordinates

```

6    0.168149063   -1.784168952   0.000000000
6    -0.996574997   -1.028729603   0.000000000
6     1.421153399   -1.184165928   0.000000000
1    -1.957087882   -1.535638321   0.000000000
1     2.312793596   -1.803775955   0.000000000
6    -0.922721287     0.353967829   0.000000000
6     1.496508195     0.194349807   0.000000000
1    -1.820389992     0.960710378   0.000000000
1     2.472222976     0.680925206   0.000000000
6     0.332265840     0.976607310   0.000000000
7     0.498596481     2.363367860   0.000000000
1     1.461296565     2.679019439   0.000000000
6    -0.468507304     3.356367053   0.000000000
8    -1.660591534     3.134946583   0.000000000
6     0.117136837     4.747458661   0.000000000
1     0.742280078     4.913988036   0.886573728
1     0.742280078     4.913988036   -0.886573728
1    -0.700693093     5.471223246   0.000000000
7     0.078598523    -3.242199885   0.000000000
8     1.125361120    -3.873777467   0.000000000
8    -1.035867445    -3.742700963   0.000000000

```



24

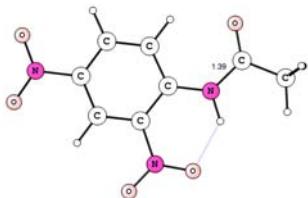
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Cartesian Coordinates

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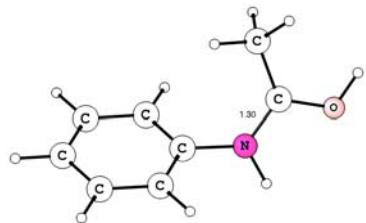
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6    1.268684538   2.096099214   0.000000000
6    -1.079397342   2.581450864   0.000000000
1    2.304165806   2.433075376   0.000000000
1    -1.902323962   3.294211939   0.000000000
6    1.010225430   0.730562727   0.000000000
6    -1.354434445   1.222686859   0.000000000
1    1.814864613   0.004199168   0.000000000
1    -2.389431112   0.876011466   0.000000000
6    -0.314984625   0.288435643   0.000000000
1    0.457225326   4.093928196   0.000000000
7    -0.676635058   -1.071093414   0.000000000
1    -1.673484744   -1.243657309   0.000000000
6    0.136599433   -2.179428237   0.000000000
8    1.352286294   -2.137127963   0.000000000
6    -0.607332403   -3.494465391   0.000000000
1    -0.300161051   -4.069061624   -0.880529246
1    -0.300161051   -4.069061624   0.880529246
1    -1.699465950   -3.403017193   0.000000000

```



25

| Charge: 0 | E: -848.7912512 H | Imag. Freq.: 0 | Cartesian Coordinates: | | |
|-----------|-------------------|----------------|------------------------|--------------|--------------|
| | | | 6 | 0.450045496 | -1.958049238 |
| | | | 6 | 1.609785444 | -1.188596507 |
| | | | 6 | -0.794545203 | -1.370713843 |
| | | | 1 | 2.576658906 | -1.683820037 |
| | | | 1 | -1.694992193 | -1.976038276 |
| | | | 6 | 1.520468754 | 0.186043421 |
| | | | 6 | -0.888136668 | 0.016070548 |
| | | | 1 | 2.414519004 | 0.797618537 |
| | | | 6 | 0.271636259 | 0.839408857 |
| | | | 7 | 0.180850676 | 2.215572756 |
| | | | 1 | -0.775005418 | 2.562074673 |
| | | | 6 | 1.208045221 | 3.156720123 |
| | | | 8 | 2.388980391 | 2.882843902 |
| | | | 6 | 0.718024761 | 4.580957937 |
| | | | 1 | 1.127052671 | 5.089036039 |
| | | | 1 | 1.127052671 | 5.089036039 |
| | | | 1 | -0.371432972 | 4.687269948 |
| | | | 7 | 0.551181473 | -3.418571431 |
| | | | 8 | -0.488501627 | -4.056373687 |
| | | | 8 | 1.673211666 | -3.898725170 |
| | | | 7 | -2.253464521 | 0.549142520 |
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| | | | 8 | -2.415487422 | 1.770694702 |



26

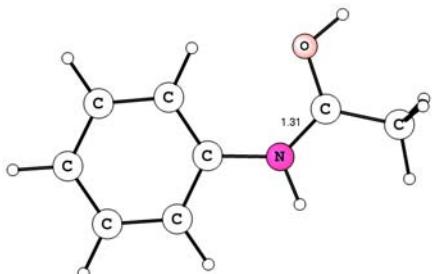
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Cartesian Coordinates

```

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6      1.335804247   2.054579612   -0.495288697
6     -0.890823820   2.520264880    0.318478330
1      2.326593904   2.401072941   -0.778608848
1     -1.631753101   3.228944555    0.680083594
6      1.016901119   0.708060322   -0.618696100
6     -1.223077525   1.176342558    0.207456821
1      1.738827251   -0.002626418   -1.019155608
1     -2.214803956   0.820178423    0.481296188
6     -0.257260405   0.288404221   -0.252211113
1      0.638471205   4.009806494    0.062332677
7     -0.615935326   -1.101819153   -0.390119038
1     -1.372093464   -1.340059530   -1.035824948
6     -0.058334677   -2.113835499    0.215269472
8     -0.520802773   -3.286240498   -0.132958632
6      1.017196704   -1.984277327    1.221710379
1      0.844104487   -2.688939781    2.044121117
1      1.986287292   -2.229615391    0.766359079
1      1.072364227   -0.968137362    1.619914116
1     -0.099130949   -4.017386720    0.351432207

```

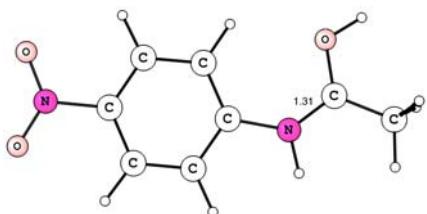


26b (less stable isomer)

Charge: +1 E: -440.306099 H Imag. Freq. 0

Cartesian Coordinates

| | | | |
|---|--------------|--------------|--------------|
| 6 | 0.211498720 | 3.025723288 | 0.037090405 |
| 6 | 1.272133320 | 2.126478814 | 0.018208170 |
| 6 | -1.098478812 | 2.557671015 | 0.053398041 |
| 1 | 2.295629098 | 2.493093741 | 0.007766077 |
| 1 | -1.933183908 | 3.253785081 | 0.069186289 |
| 6 | 1.047884410 | 0.755909975 | 0.013482307 |
| 6 | -1.343090730 | 1.194346223 | 0.049773078 |
| 1 | 1.887646849 | 0.071896339 | 0.002115800 |
| 1 | -2.369217610 | 0.825109610 | 0.061965813 |
| 6 | -0.270004657 | 0.302269987 | 0.028141561 |
| 1 | 0.406270784 | 4.095484075 | 0.040395485 |
| 7 | -0.641504772 | -1.080901632 | 0.030569247 |
| 1 | -1.645701208 | -1.223441727 | 0.111798827 |
| 6 | 0.049412832 | -2.185158663 | -0.053351523 |
| 8 | 1.348777533 | -2.093190137 | -0.163926965 |
| 6 | -0.605701370 | -3.514785578 | -0.024785512 |
| 1 | -0.357498074 | -4.074373010 | -0.936461935 |
| 1 | -0.240883640 | -4.092868788 | 0.834889717 |
| 1 | -1.694196944 | -3.444294942 | 0.047604068 |
| 1 | 1.772821992 | -2.967315597 | -0.226446438 |

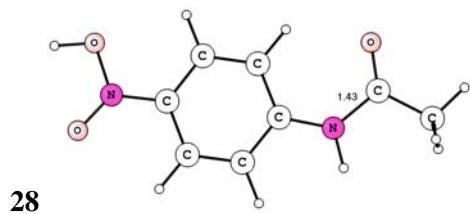


27

Charge: +1 E: -644.7083593 H Imag. Freq. 0

Cartesian Coordinates

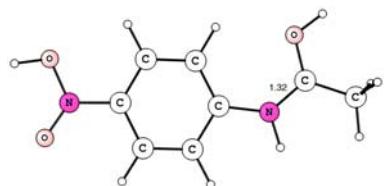
| | | | |
|---|--------------|--------------|--------------|
| 6 | -0.103230916 | -1.806534457 | 0.000000000 |
| 6 | -1.157450095 | -0.908370566 | 0.000000000 |
| 6 | 1.221317237 | -1.399335635 | 0.000000000 |
| 1 | -2.176881294 | -1.283525205 | 0.000000000 |
| 1 | 2.014852275 | -2.140918137 | 0.000000000 |
| 6 | -0.893184386 | 0.453821336 | 0.000000000 |
| 6 | 1.490514104 | -0.042205838 | 0.000000000 |
| 1 | -1.717110103 | 1.156187878 | 0.000000000 |
| 1 | 2.525067799 | 0.300661199 | 0.000000000 |
| 6 | 0.436662148 | 0.874258798 | 0.000000000 |
| 7 | 0.840906933 | 2.248092594 | 0.000000000 |
| 1 | 1.851435507 | 2.368810794 | 0.000000000 |
| 6 | 0.169244128 | 3.369900879 | 0.000000000 |
| 8 | -1.133277058 | 3.306349917 | 0.000000000 |
| 6 | 0.856733801 | 4.682432703 | 0.000000000 |
| 1 | 0.561210396 | 5.257694415 | -0.887743130 |
| 1 | 0.561210396 | 5.257694415 | 0.887743130 |
| 1 | 1.945796395 | 4.587881961 | 0.000000000 |
| 7 | -0.400846775 | -3.255634681 | 0.000000000 |
| 8 | 0.552985389 | -4.009818482 | 0.000000000 |
| 8 | -1.574138200 | -3.574537169 | 0.000000000 |
| 1 | -1.546575621 | 4.188828094 | 0.000000000 |



Charge: +1 E: -644.7156978 H Imag. Freq. 0

Cartesian Coordinates

| | | | |
|---|--------------|--------------|--------------|
| 6 | -0.096357415 | -1.767942232 | 0.000000000 |
| 6 | -1.141528580 | -0.813580728 | 0.000000000 |
| 6 | 1.262456964 | -1.369773784 | 0.000000000 |
| 1 | -2.178733059 | -1.134897038 | 0.000000000 |
| 1 | 2.046761711 | -2.121876103 | 0.000000000 |
| 6 | -0.839016923 | 0.518635591 | 0.000000000 |
| 6 | 1.555510030 | -0.039544417 | 0.000000000 |
| 1 | -1.623871252 | 1.265517909 | 0.000000000 |
| 1 | 2.594845826 | 0.283905759 | 0.000000000 |
| 6 | 0.520064643 | 0.936853064 | 0.000000000 |
| 7 | 0.891682400 | 2.242699809 | 0.000000000 |
| 1 | 1.892751682 | 2.419510412 | 0.000000000 |
| 6 | 0.060879902 | 3.407638684 | 0.000000000 |
| 8 | -1.138207914 | 3.322626148 | 0.000000000 |
| 6 | 0.848540028 | 4.679797404 | 0.000000000 |
| 1 | 1.491407768 | 4.745442183 | 0.887189583 |
| 1 | 1.491407768 | 4.745442183 | -0.887189583 |
| 1 | 0.153801380 | 5.522212526 | 0.000000000 |
| 7 | -0.359182077 | -3.113891497 | 0.000000000 |
| 8 | 0.450867397 | -4.004326911 | 0.000000000 |
| 8 | -1.671027133 | -3.433500913 | 0.000000000 |
| 1 | -1.682462683 | -4.417086478 | 0.000000000 |

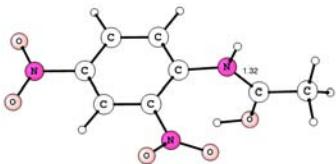


29

Charge: +2 E: -644.929194 H Imag. Freq. 0

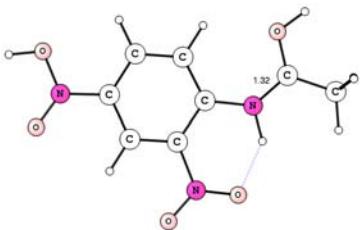
Cartesian Coordinates

| | | | |
|---|--------------|--------------|--------------|
| 6 | -0.096522489 | -1.784531848 | 0.000000000 |
| 6 | -1.159823453 | -0.872789434 | 0.000000000 |
| 6 | 1.246044467 | -1.381487902 | 0.000000000 |
| 1 | -2.193087997 | -1.208246612 | 0.000000000 |
| 1 | 2.050824058 | -2.112811541 | 0.000000000 |
| 6 | -0.874376227 | 0.479648649 | 0.000000000 |
| 6 | 1.515578191 | -0.031433211 | 0.000000000 |
| 1 | -1.694415671 | 1.186648249 | 0.000000000 |
| 1 | 2.552686241 | 0.300634922 | 0.000000000 |
| 6 | 0.463262196 | 0.897511821 | 0.000000000 |
| 7 | 0.867986593 | 2.259434627 | 0.000000000 |
| 1 | 1.878566961 | 2.390717730 | 0.000000000 |
| 6 | 0.183671621 | 3.392791283 | 0.000000000 |
| 8 | -1.106807957 | 3.312153332 | 0.000000000 |
| 6 | 0.873597742 | 4.698412114 | 0.000000000 |
| 1 | 0.573471102 | 5.275651911 | -0.886685385 |
| 1 | 0.573471102 | 5.275651911 | 0.886685385 |
| 1 | 1.963160396 | 4.608519949 | 0.000000000 |
| 7 | -0.340381072 | -3.180229159 | 0.000000000 |
| 8 | 0.499749324 | -4.019235273 | 0.000000000 |
| 8 | -1.625708196 | -3.507336953 | 0.000000000 |
| 1 | -1.548799669 | 4.185768460 | 0.000000000 |
| 1 | -1.667715417 | -4.497314611 | 0.000000000 |



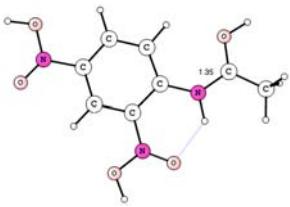
30

| <u>Charge:</u> | <u>+1</u> | <u>E:</u> | <u>-849.1075907 H</u> | <u>Imag. Freq. 0</u> | Cartesian Coordinates |
|----------------|-----------|-----------|-----------------------|----------------------|---|
| | | | | | 6 0.409230726 2.907951578 0.010835794 |
| | | | | | 6 1.345544441 2.083399366 -0.591064620 |
| | | | | | 6 -0.815835332 2.448333247 0.460376460 |
| | | | | | 1 2.294479291 2.480425947 -0.944978408 |
| | | | | | 1 -1.515894871 3.143823620 0.915856040 |
| | | | | | 6 1.038465555 0.740790543 -0.722123062 |
| | | | | | 6 -1.121128784 1.100011763 0.301688144 |
| | | | | | 1 -2.088185540 0.711453545 0.614534234 |
| | | | | | 6 -0.196106029 0.239715285 -0.277312876 |
| | | | | | 7 -0.579804776 -1.128567579 -0.497579549 |
| | | | | | 1 -1.092682435 -1.346021048 -1.350489500 |
| | | | | | 6 -0.206617220 -2.148610519 0.246244828 |
| | | | | | 8 0.450732280 -1.998516272 1.346125850 |
| | | | | | 6 -0.504461452 -3.537446410 -0.141197215 |
| | | | | | 1 0.422942537 -3.963775733 -0.551930725 |
| | | | | | 1 -0.772313437 -4.126218116 0.741569738 |
| | | | | | 1 -1.291131608 -3.604986445 -0.896802540 |
| | | | | | 1 0.738269286 -1.078734026 1.514434075 |
| | | | | | 7 0.738419326 4.347295721 0.175599077 |
| | | | | | 8 1.834206150 4.699331060 -0.209595472 |
| | | | | | 8 -0.118670228 5.041549601 0.682569609 |
| | | | | | 7 2.060746173 -0.134589617 -1.327444525 |
| | | | | | 8 2.076291455 -1.301681462 -0.954631590 |
| | | | | | 8 2.813348190 0.369547373 -2.126333370 |



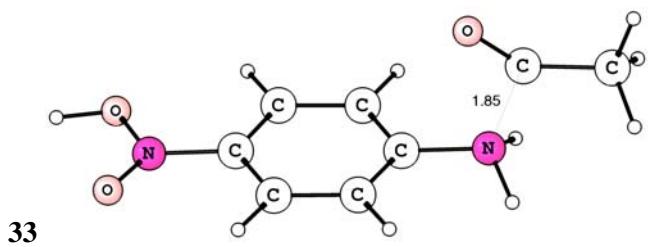
31

| <u>Charge:</u> +2 | <u>E:</u> -849.3211556 H | <u>Imag. Freq.:</u> 0 | Cartesian Coordinates | | |
|-------------------|--------------------------|-----------------------|------------------------------|--------------|--------------|
| | | | 6 | -2.011422000 | -0.447150000 |
| | | | 6 | -1.248747000 | -1.620356000 |
| | | | 6 | -1.427102000 | 0.819724000 |
| | | | 1 | -1.715553000 | -2.601836000 |
| | | | 1 | -2.019509000 | 1.734174000 |
| | | | 6 | 0.128788000 | -1.512991000 |
| | | | 6 | -0.053429000 | 0.908226000 |
| | | | 1 | 0.718430000 | -2.421131000 |
| | | | 6 | 0.758204000 | -0.258144000 |
| | | | 7 | 2.154203000 | -0.099064000 |
| | | | 1 | 2.415784000 | 0.904256000 |
| | | | 6 | 3.155983000 | -0.964364000 |
| | | | 8 | 2.878321000 | -2.227760000 |
| | | | 6 | 4.551804000 | -0.484491000 |
| | | | 1 | 4.626250000 | 0.605918000 |
| | | | 1 | 5.075566000 | -0.890112000 |
| | | | 1 | 5.077332000 | -0.850642000 |
| | | | 7 | -3.431803000 | -0.489526000 |
| | | | 8 | -3.930633000 | -1.715317000 |
| | | | 8 | -4.139763000 | 0.461419000 |
| | | | 7 | 0.482754000 | 2.304108000 |
| | | | 8 | 1.701931000 | 2.448142000 |
| | | | 8 | -0.321782000 | 3.194972000 |
| | | | 1 | -4.918597000 | -1.626248000 |
| | | | 1 | 3.675146000 | -2.797390000 |
| | | | | | -0.046127000 |



32

| <u>Charge:</u> +3 | <u>E:</u> -849.390648 H | <u>Imag. Freq.</u> 0 | Cartesian Coordinates | | |
|-------------------|-------------------------|----------------------|------------------------------|--------------|--------------|
| | | | 6 | -2.000227000 | -0.495118000 |
| | | | 6 | -1.193133000 | -1.639915000 |
| | | | 6 | -1.462817000 | 0.778427000 |
| | | | 1 | -1.625229000 | -2.640179000 |
| | | | 1 | -2.110039000 | 1.655065000 |
| | | | 6 | 0.186637000 | -1.498038000 |
| | | | 6 | -0.066334000 | 0.909260000 |
| | | | 1 | 0.784445000 | -2.401120000 |
| | | | 6 | 0.806515000 | -0.242323000 |
| | | | 7 | 2.199337000 | -0.092381000 |
| | | | 1 | 2.539867000 | 0.868813000 |
| | | | 6 | 3.206082000 | -0.993923000 |
| | | | 8 | 2.891300000 | -2.235090000 |
| | | | 6 | 4.602776000 | -0.535370000 |
| | | | 1 | 4.711329000 | 0.552172000 |
| | | | 1 | 5.120933000 | -0.965875000 |
| | | | 1 | 5.128286000 | -0.909854000 |
| | | | 7 | -3.445875000 | -0.590797000 |
| | | | 8 | -3.878092000 | -1.826892000 |
| | | | 8 | -4.167461000 | 0.342737000 |
| | | | 7 | 0.445426000 | 2.238621000 |
| | | | 8 | 1.602974000 | 2.527474000 |
| | | | 8 | -0.471975000 | 3.174358000 |
| | | | 1 | -4.877148000 | -1.818822000 |
| | | | 1 | -0.016778000 | 4.063075000 |
| | | | 1 | 3.661161000 | -2.850077000 |
| | | | | | -0.065417000 |



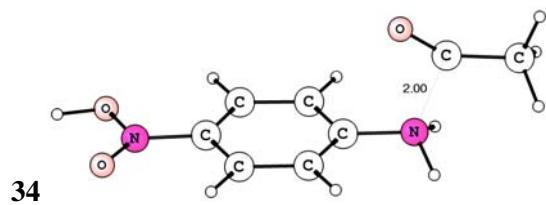
Charge: +2 E: -644.8956204 H Imag. Freq. 0

Cartesian Coordinates

```

6    0.418034466   2.883372410   0.044744363
6    1.238923521   2.142557778   -0.816326036
6    -0.750972910   2.367150368   0.620317918
1    2.142817311   2.565315100   -1.246074192
1    -1.357983095   2.974212752   1.288160155
6    0.862397268   0.844383785   -1.108926448
6    -1.109804227   1.069330147   0.314363355
1    1.481199791   0.246193276   -1.775959115
1    -2.013867785   0.645596123   0.748953039
6    -0.310963519   0.326725920   -0.557267506
7    -0.672884400   -1.038084536   -0.833175210
1    -1.692257813   -1.166061259   -0.844272451
6    0.011669700   -2.180936165   0.451750985
8    0.606252406   -1.589957934   1.246758612
6    -0.401419536   -3.540204783   0.097136232
1    0.010933575   -4.226184781   0.846555230
1    -1.496355850   -3.622794807   0.090067573
1    -0.025801438   -3.814755047   -0.897004717
7    0.745431161   4.225620347   0.378069222
8    1.852933525   4.670827832   -0.194907826
8    0.110792179   4.921360682   1.099330864
1    -0.324081425   -1.349152316   -1.747914277
1    1.977418137   5.607064074   0.106528709

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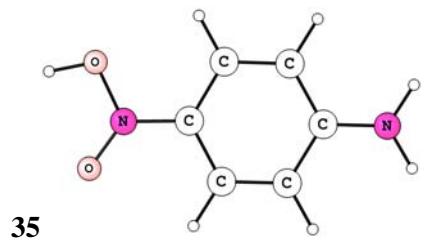
Charge: +2 E: -644.895437 H Imag. Freq.: 1

Cartesian Coordinates

```

6    0.432499057   2.869067926   0.044111716
6    1.248341254   2.128341995   -0.823729316
6    -0.721907497   2.340965015   0.640867667
1    2.139327779   2.559299015   -1.271928405
1    -1.326247125   2.946825240   1.312095043
6    0.881852487   0.826140721   -1.102609190
6    -1.070872496   1.039111674   0.347873702
1    1.494209444   0.233085044   -1.779988604
1    -1.966588077   0.610250219   0.794622252
6    -0.280719518   0.294014571   -0.534512924
7    -0.642133057   -1.058055278   -0.808630657
1    -1.659474407   -1.184821785   -0.824786067
6    0.059229067   -2.278716483   0.616554445
8    0.582987916   -1.633688726   1.406526353
6    -0.333014027   -3.613940272   0.189048360
1    0.030788222   -4.325322862   0.942305322
1    -1.425515856   -3.685729023   0.110658490
1    0.109046904   -3.851482390   -0.786844732
7    0.745231068   4.214674607   0.356703134
8    1.837276085   4.671227480   -0.240790345
8    0.114148452   4.911987738   1.081766391
1    -0.277287168   -1.380244581   -1.710610934
1    1.949310461   5.612084022   0.049048578

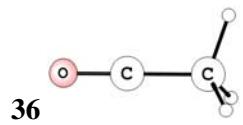
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Charge: +1 E: -492.1532721 H Imag. Freq.: 0

Cartesian Coordinates

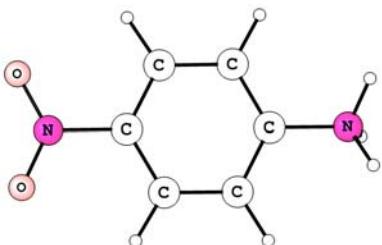
| | | | |
|---|--------------|--------------|-------------|
| 6 | -0.023023686 | -0.613637167 | 0.000000000 |
| 6 | 1.223000014 | 0.067200732 | 0.000000000 |
| 6 | -1.250443186 | 0.100114333 | 0.000000000 |
| 1 | 2.154009514 | -0.491164667 | 0.000000000 |
| 1 | -2.187767586 | -0.449894768 | 0.000000000 |
| 6 | 1.232842814 | 1.427718632 | 0.000000000 |
| 6 | -1.231594286 | 1.459470833 | 0.000000000 |
| 1 | 2.177114914 | 1.968241333 | 0.000000000 |
| 1 | -2.162698086 | 2.022236632 | 0.000000000 |
| 6 | 0.009875214 | 2.161542832 | 0.000000000 |
| 7 | 0.027019514 | 3.492629033 | 0.000000000 |
| 1 | -0.829333686 | 4.033922333 | 0.000000000 |
| 7 | -0.088554186 | -1.976549968 | 0.000000000 |
| 8 | 1.112311114 | -2.602483068 | 0.000000000 |
| 8 | -1.087592686 | -2.652664867 | 0.000000000 |
| 1 | 0.896330614 | 4.013034633 | 0.000000000 |
| 1 | 0.883481014 | -3.558407467 | 0.000000000 |



Charge: +1 E: -152.8298682 H Imag. Freq.: 0

Cartesian Coordinates

| | | | |
|---|--------------|---------------|-------------|
| 6 | 0.460575213 | -8.514934011 | 3.337030391 |
| 8 | 0.480541707 | -7.493533799 | 2.872230756 |
| 6 | 0.435753430 | -9.808128313 | 3.925456073 |
| 1 | -0.454315725 | -10.347764018 | 3.565896017 |
| 1 | 1.348462694 | -10.351344813 | 3.634087141 |
| 1 | 0.394249601 | -9.701568906 | 5.020753659 |



37:

Charge: +1 E: -492.1301197 H Imag. Freq.: 0

Cartesian Coordinates

| | | | |
|---|--------------|--------------|--------------|
| 6 | -0.011330646 | -0.567746900 | 0.000629835 |
| 6 | 1.212738025 | 0.081963121 | -0.003765588 |
| 6 | -1.224020405 | 0.103138612 | -0.002994760 |
| 1 | 2.130269535 | -0.499813828 | -0.004940233 |
| 1 | -2.151305325 | -0.463096823 | -0.003694357 |
| 6 | 1.228253506 | 1.470665246 | -0.009558202 |
| 6 | -1.215724197 | 1.491866654 | -0.008798013 |
| 1 | 2.175389538 | 2.008669211 | -0.012460288 |
| 1 | -2.153444304 | 2.046141114 | -0.010945680 |
| 6 | 0.011908109 | 2.134398250 | -0.011405604 |
| 7 | -0.024240982 | -2.051608062 | 0.005729624 |
| 8 | 1.056791356 | -2.604999384 | 0.007586308 |
| 8 | -1.115107928 | -2.585589940 | 0.008494164 |
| 7 | 0.024919465 | 3.624304739 | 0.007083439 |
| 1 | 0.033385175 | 4.000925282 | 0.966331190 |
| 1 | 0.852822430 | 4.000248910 | -0.474443962 |
| 1 | -0.801191755 | 4.015161027 | -0.4657207 |